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STUDY OF FLAME ACCELERATION IN CLOSED AND HALF-OPEN DUCTS

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Abstract. *The objective of the present study is to validate the available theory of early-stage flame acceleration in closed and half-open ducts. To achieve this goal, first, a review of the flame propagation inside ducts was presented. Afterward, several results from published works related to flame acceleration in ducts were collected and analyzed. The study of flame propagation inside ducts is relevant to the safety of industrial facilities. The flame propagation can be classified into deflagrations and detonations. The deflagrations occur at a subsonic speed ($M < 1$), while detonations occur at supersonic speed ($M > 1$). The present work is focused on deflagrations. The flame acceleration develops with a finger shape flame front, growing exponentially over time. The mechanism of the flame front inversion will be discussed and outlined. Thus, parameters as the equivalence ratio and the type of fuel will be considered for analysis. The theory for the initial stages of flame acceleration for low Mach numbers, proposed by Valiev, was validated with experimental data published in recent works. The results show that the available theory is accurate for the determination of the maximum flame speed by using experimental data of flame tip position at the time at which the flame skirt touches the sidewalls. A relevant parameter in flame propagation is the maximum calculated flame tip velocity ratio to the experimental value. A good correlation was obtained between this parameter, the laminar flame velocity and the time at which the flame skirt touches the sidewalls.*

Keywords: *Flame propagation, closed ducts, half-open ducts, premixed flames, flame front inversion*

1. INTRODUCTION

The study of flame propagation inside ducts is very important for practical applications such as the burning process of typical internal combustion engines (Bychkov, *et al.*, 2007). In this sense, much research has been carried out since the beginning of the century analyzing the behavior of premixed flames inside ducts and tubes. In the meantime, there is a worldwide interest in renewable energies and alternative fuels for energy sustainability. Thus, the knowledge of the combustion characteristics of these fuels and the flame propagation is vital for the use of alternative fuels such as syngas and biogas.

The flame propagation can be classified into deflagrations and detonations. The deflagrations occur at subsonic speeds ($M < 1$), while detonations occur at supersonic speeds ($M > 1$) (Kuo, 2005). This important factor is associated with the safety of industrial facilities (Oran, *et al.*, 2019). Therefore, by improving the understanding of the behavior of the acceleration of flames, it is possible to prevent and control industrial disasters that can cause financial losses, and above all, take lives.

In the first experimental studies on flame propagation, in the mid-1930s, it was discovered by Ellis that the shape of the flame front changes from convex to concave when the duct length to diameter ratio (aspect ratio) is greater than two (Ellis, 1928). Years later, Salamandra called this flame a tulip flame (Salamandra, *et al.*, 1959). The tulip flame has a particular shape of the flame front with an inverted curvature, which can often be observed during the propagation of the laminar flame, both in closed and half-open ducts (Yang, *et al.*, 2019b). In this way, some experimental studies and numerical simulations were carried out by different authors to try to explain this inversion of the flame front (Ponizy, *et al.*, 2014) (Yu, *et al.*, 2018). Early research reports that this reversal of the flame front may be a result of the interaction between the flame and a shock wave. However, shock waves are hardly observed until the tulip flame forms.

Ponizy *et al.* (2014) studied the formation of the tulip flame in closed ducts by using PIV images and direct visualization of the process. From the results obtained, the authors concluded that the tulip flame is a purely hydrodynamic phenomenon generated by the competition between the flow of burnt and unburnt gases resulting in the inversion of the flame front (Ponizy, *et al.*, 2014).

According to Bychkov *et al.* (2007), the acceleration happens due to the increasing flame front's surface, which develops with a finger-shaped flame front, growing exponentially over time. This increase in the surface of the flame front occurs until the flame skirt touches the sidewalls of the duct and thus its surface starts to decrease. At this moment there is a deceleration of the flame front, which can cause the formation of tulip flames (Bychkov, *et al.*, 2007).

Valiev *et al.* studied the initial acceleration process of a fast-burning flame, with mixtures of hydrogen and oxygen, using the Schlieren technique, and observed that the rate of flame acceleration decreases significantly with the increase in the initial Mach number (Valiev, *et al.*, 2013). In this same work, the theory for the initial stages of flame acceleration for low Mach numbers was presented. The finger flame acceleration theory can demonstrate an important quantitative and qualitative correlation in deflagrations. However, this theory has not been validated with the recently published experimental data.

Jin *et al.* (2017) studied the propagation of premixed flames of natural gas, methane, and acetylene in a closed duct. It was observed that the composition of the fuel has a significant influence on the speed of flame propagation and on the shape of the flame. A small amount of ethane and propane added found in the natural gas mixture was responsible for accelerating the flame and increasing the pressure in comparison to pure methane (Jin, *et al.*, 2017). On the other hand, due to the greater chemical reactivity, acetylene has a higher flame propagation speed than natural gas and methane. However, the results obtained in this research were not used to evaluate the theory developed by Valiev *et al.* (2013).

Yu *et al.* (2018) studied experimentally the deflagration of premixed hydrogen, carbon monoxide, and air flames inside a closed duct. The results obtained in this research showed the formation of the tulip flame for equivalence ratios from 1.0 to 3.0 and for hydrogen mole fractions from 0.1 to 0.9. However, the distorted tulip flame was only formed for cases where the hydrogen mole fraction was greater than 0.5 in all equivalence ratios. Likewise, the hydrogen fractions in the mixture have a significant influence on the flame shape and flame propagation speed (Yu, *et al.*, 2018). For the considered gas composition, the minimum flame propagation time can be obtained with an equivalence ratio of 1.5. In addition, the time of formation of the flat flame is directly influenced by the laminar flame speed. However, the results of this research have not been used to evaluate the available theory by Valiev *et al.* (2013).

The behavior of the premixed flames of hydrogen, carbon monoxide, and air mixtures, was experimentally investigated in a half-open duct by Yang *et al.* (2019a). As the hydrogen fraction increases, there is a greater stretch of the flame front at the stage where the flame skirt touches the sidewalls. The plane flame will form after this stretch process as usual (Yang, *et al.*, 2019a). This provides evidence that flame inversion is a purely hydrodynamic phenomenon. However, these results have not been compared to the theory of Valiev *et al.* (2013).

Yang *et al.* (2019b) performed a comparison between the behavior of the flame propagation of premixed flames of syngas and air inside a closed duct (C-D) and inside a half-open (HO-D) duct. With this study, it was confirmed that a flame propagates differently in C-D and HO-D ducts. Sequential formations of the distorted tulip flame are observed in the C-D configuration, while in the HO-D configuration the distorted tulip forms only once. Nevertheless, the time when the flame skirt touches the sidewalls (τ_{wall}) is almost the same for both duct configurations (Yang, *et al.*, 2019b). The results obtained in this work were also not examined by applying the theory by Valiev *et al.* (2013).

Recently, Luo *et al.* (2020) studied the deflagration characteristics of methane and ethane in air inside a closed duct. The results obtained in this research show that, with the increase of the ethane volume fraction in the mixture, the reaction rate and the explosion intensity of the premixed gas increase (Luo, *et al.*, 2020). However, as in the works presented above, the results obtained were also not used to validate the theory presented by Valiev *et al.* (2013).

From this, the main objective of the present work is to validate the available theory of Valiev *et al.* (2013) with experimental data published after the publication of that theory. Thus, extensive validation of Valiev's flame acceleration theory will be performed using experimental data published in scientific articles in the last five years relating the parameters of the time at which the flame touches the sidewalls (τ_w) and the maximum flame tip velocity ($U_{tip,max}$).

2. METHODOLOGY

Mendiburu *et al.* (2019) presented the four main phases in the process of flame propagation inside a closed duct. These phases are represented in Figure 1. In the first phase, there is a free spherically expanding flame with a constant speed, this phase happens right after the ignition. In the second phase, the flame takes the form of a finger-shaped flame and thus the surface area of the flame increases rapidly. At the end of this phase, the flame skirt reaches the sidewalls of the duct and at this point, we have τ_w as presented in the work by Valiev *et al.* (2013). In the third phase, the formation of the flat flame occurs and at that moment there is a deceleration of the flame propagation. In the fourth phase, the flame front is inverted, causing the tulip flame phenomenon.

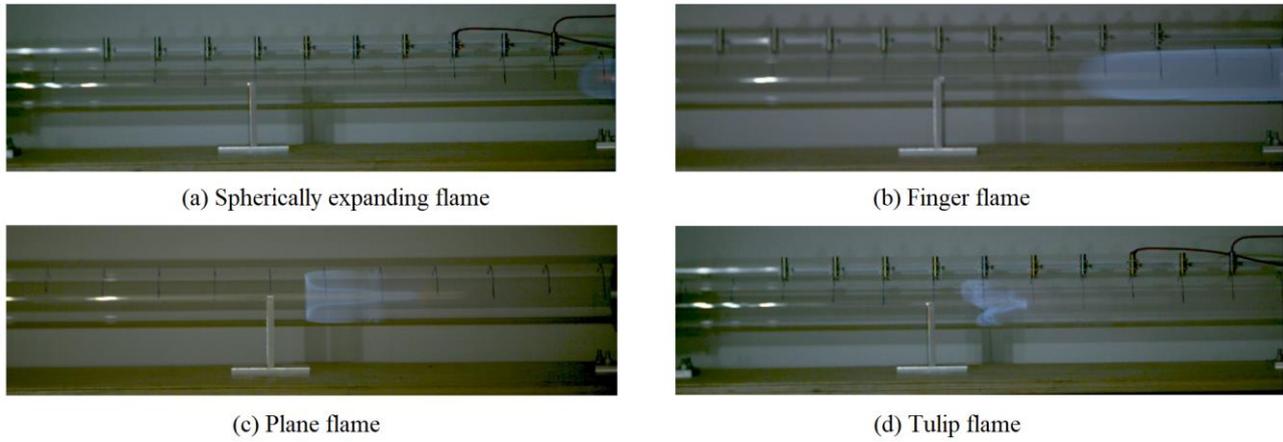


Figure 1. Schematic representation of the phases of the flame propagation inside a duct.
Mendiburu *et. al.* (2019)

The experimental data of the time at which the flame touches the sidewalls (τ_w) and the maximum flame tip velocity ($U_{tip,max}$) will be obtained from experimental works related to the tulip flame phenomenon, that were published within the last five years. All experimental data, including another important parameter, the dimensionless axial location of the flame tip touch the sidewalls ($\xi_{tip,wall}$), were collected from the experimental articles by Jin *et. al.* (2017), Yu *et. al.* (2018), Yang *et. al.* (2019a), Yang *et. al.* (2019b), Yang *et. al.* (2020), and Luo *et. al.* (2020). In most experimental works the value of $\xi_{tip,wall}$ was presented in graphical form. To find the value of this parameter, the GetData Graph Digitizer software (GetData Graph Digitizer, 2021) was used. The value of $\xi_{tip,wall}$ was obtained by looking for the points of the graphs that related the time when the flame touches the sidewalls to the flame tip position at that time. The thermodynamic properties and laminar flame velocities were determined by using the Cantera software (Cantera, 2021). The initial pressure and temperature were 101325 Pa and 298,15 K, respectively. The chemical kinetic mechanism used to obtain the laminar flame velocities was the San Diego Mechanism (San Diego, 2021).

As already mentioned, the theory described by Valiev *et. al.* (2013) was applied. This theory describes the early stages of axial flame acceleration for planar geometry. The theory considers a laminar, compressible, isentropic flow, and adiabatic duct walls. For simplicity, in this work the maximum experimental flame tip velocity is represented by U_{exp} , the maximum calculated flame tip velocity is U_{calc} . The dimensionless axial location of the flame tip is ξ_{tip} . At the time when the flame skirt touches the sidewalls, the dimensionless experimental axial location of the flame tip is ξ_{exp} and the dimensionless calculated axial location of the flame tip is ξ_{calc} .

Valiev *et. al.* (2013) made some simplifying assumptions, the most important are: a) Infinitely thin flame front, b) Potential flow in the unburned mixture, c) Potential flow for the burned gases close to the end wall, d) The flow is planar in the vicinity of the centerline; thus, the flow can be considered potential, e) The flow ahead of the flame is isentropic, f) the duct is half-open. The analysis performed by Valiev *et. al.* (2013), for a planar geometry, leads to the differential equation shown in Eq. (1).

$$\frac{d\xi}{d\tau} = -Ma\gamma(\theta - 1)^2\xi^2 + \sigma_{1,pl}\xi^2 + \theta_1 \quad (1)$$

The time at which the flame skirt touches the sidewalls of the duct is given by Eq. (2).

$$\tau_w = \frac{\ln\theta}{\theta - 1} \quad (2)$$

The solution of the differential equation, Eq. (1), provides the dimensionless axial position of the flame tip, as shown in Eq. (3).

$$\xi = \frac{2\theta_1[\exp(\sigma_2\tau) - 1]}{(\sigma_2 - \sigma_{1,pl})\exp(\sigma_2\tau) + (\sigma_2 + \sigma_{1,pl})} \quad (3)$$

The maximum flame tip velocity is given by Eq. (4).

$$\frac{U}{S_L} = -Ma\gamma(\theta - 1)^2\xi^2_w + \sigma_{1,pl}\xi_w + \theta_1 \quad (4)$$

The auxiliary parameters are given by Eq. (5), Eq. (6), and Eq. (7).

$$\sigma_{1,pl} = (\theta - 1)[1 - Ma(\theta + 2(\gamma - 1)(\theta - 1))] \quad (5)$$

$$\theta_1 = \theta - Ma(\gamma - 1)(\theta - 1)^2 \quad (6)$$

$$\sigma_2 = \sqrt{\sigma_{1,pl}^2 + 4Ma\gamma\theta_1(\theta - 1)^2} \quad (7)$$

where ξ , τ_w , and U are the dimensionless axial coordinate, the dimensionless time, and the maximum flame tip velocity, respectively. While θ , γ , and Ma are the gas expansion ratio, the ratio of heat capacities, and the initial flame propagation Mach number, respectively.

Eq. (2) occurs at the moment represented by Figure 1 (b) and the maximum flame tip velocity, Eq. (4), can be represented between the instants depicted in Figure 1 (c) and Figure 1 (d). Thus, in this work, we will use the Eq. (4) of maximum flame tip velocity considering a ξ_{calc} by Eq. (3) and ξ_{exp} extracted from the graphs of the experimental articles.

3. RESULTS AND DISCUSSION

In the first part of this study, $U_{calc}(\xi_{exp})$, $U_{calc}(\xi_{calc})$, and all U_{exp} data collected from the experimental works by Jin *et al.* (2017), Yu *et al.* (2018), and Yang *et al.* (2020), were plotted as a function of equivalence ratio for some air-fuel mixtures in Figure 2. It is observed that, in Figure 2 (a), for methane, the values of U_{exp} and $U_{calc}(\xi_{exp})$ denotes a good approximation, while the results using ξ_{calc} are more distant. In Figure 2 (b), the fuel is acetylene, it can be observed that all the analyzed maximum velocities have a good agreement up to the equivalence ratio of 1.30. Above this equivalence ratio, only U_{exp} and $U_{calc}(\xi_{exp})$ follow the same trend. Figure 2 (c) shows the fuel mixture of 0.3H₂+0.7CO. In this case, the equivalence ratio ranged from 1.00 to 3.00. It can be noticed that in carbon monoxide and hydrogen mixtures all parameters follow the same trend. Nevertheless, the parameters of U_{exp} and $U_{calc}(\xi_{exp})$ have a better approximation among them. Finally, a fuel mixture of 0.5H₂+0.5CO is depicted in Figure 2(d). In this case, the equivalence ratio ranged from 0.80 to 3.00. It can be noticed that with the increasing hydrogen fraction in the mixture, all parameters continue to follow the same trend. However, the agreement among them decreases considerably. For the mixtures of Figure 2 (a), (b), and (c) the results of U_{exp} and $U_{calc}(\xi_{exp})$ have a good agreement quantitatively and qualitatively.

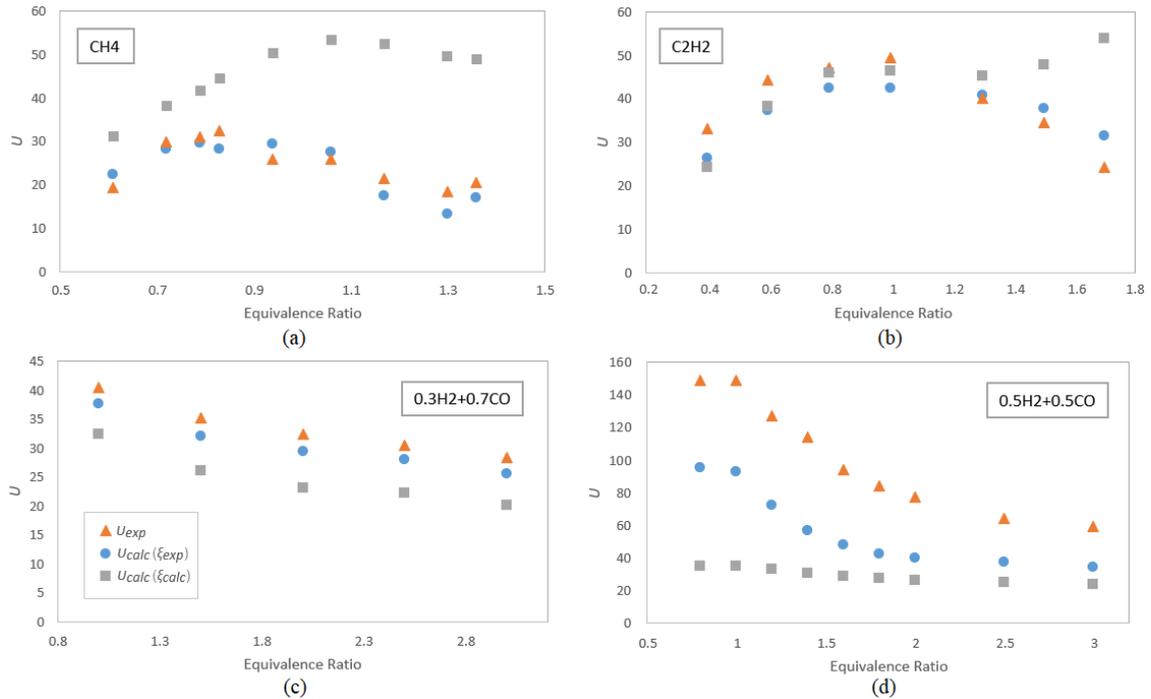


Figure 2. Maximum tip flame velocity (U) versus equivalence ratio for each fuel.

Therefore, from the results obtained above, it can be observed that when ξ_{exp} was used to obtain U_{calc} , the results were more consistent with the experimental data in comparison to the calculations performed with ξ_{calc} . Therefore, the determination of ξ_{calc} by the theory of Valiev et al. is a key step that causes most of the divergences with the experimental values of the maximum flame tip velocity. In the following analysis, only the values of $U_{calc}(\xi_{exp})$ will be considered.

In Figure 3 the ratios U_{calc}/U_{exp} , obtained for deflagrations of H₂+CO mixtures inside closed and half-open ducts, are depicted as a function of the laminar flame speed. The data were correlated, and a Person's correlation coefficient was determined. In Figure 3 (a) the data correspond to a closed duct, an equivalence ratio of 0.80 and hydrogen fractions ranging from 0.1 to 0.9. The value of the Person's coefficient (R^2) was 0.8731, which is a good correlation between the parameters. Similarly, in Figure 3 (b) the data depicted was obtained in a closed duct, the equivalence ratio ranged from 1.00 to 3.00, and the hydrogen fractions ranged from 0.1 to 0.9. It is observed that the value of the Person's coefficient (R^2) was 0.7076, which means that there is a good correlation between the parameters. Figure 3(c) shows data obtained inside a half-open duct, as in the first case, the equivalence ratio was 0.80, and the hydrogen fractions ranged from 0.1 to 0.9. The value of the Person's coefficient (R^2) was 0.9213, which is a very good correlation between the parameters. Figure 3(d) depicts the data for a half-open duct, the equivalence ratio was 1.20, and the hydrogen fractions ranged from 0.1 to 0.9. The value of the Person's coefficient (R^2) was 0.9855, which shows an excellent correlation between the parameters. Finally, Figure 3 (e) shows data for a half-open duct, the equivalence ratio was 0.80, and the hydrogen fractions ranged from 0.1 to 0.9. It is observed that the value of the Person's coefficient (R^2) was 0.9754, which denotes an excellent correlation between the parameters.

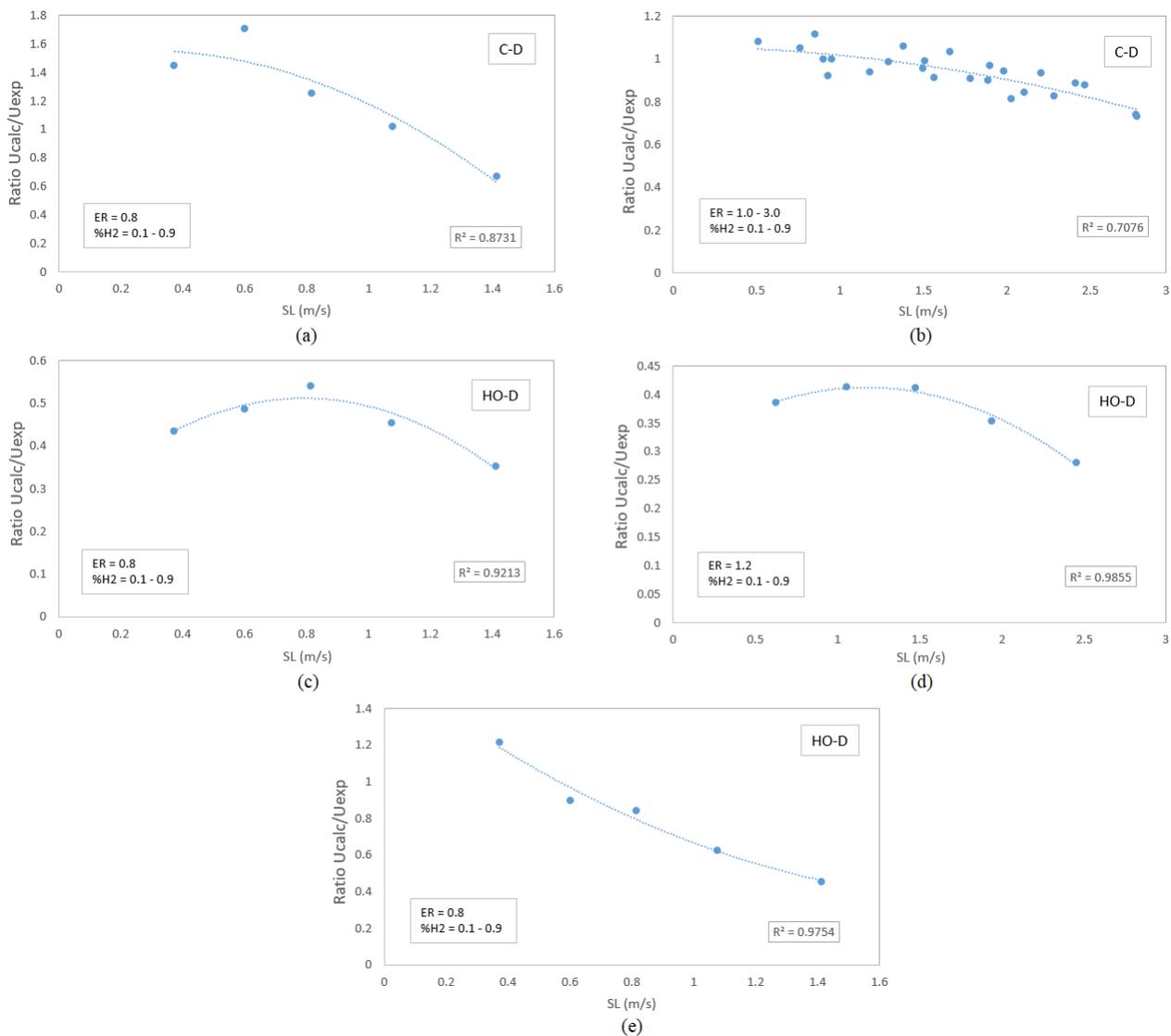


Figure 3. The ratio of maximum velocity U_{calc}/U_{exp} as a function of the laminar flame velocity for hydrogen and carbon monoxide mixtures in closed ducts (a-b) and half-open ducts (c-e).

From the results presented in Figure 3, it can be observed that the best correlations were obtained for half-open ducts for hydrogen and carbon monoxide mixtures with hydrogen fractions ranging from 0.1 to 0.9 and equivalence ratios of 0.8 and 1.2. The theory developed by Valiev *et. al.* (2013) did not consider the compression caused by the closed duct configuration. Therefore, the results are coherent with the theoretical boundary conditions. Nevertheless, the theory shows acceptable agreement when applied to closed ducts.

Another important comparison is performed by considering the ratio of the maximum flame tip velocity U_{calc}/U_{exp} , and the time at which the flame skirt touches the sidewalls (τ_w). Figure 4 shows the data for the ratio U_{calc}/U_{exp} as a function of the calculated time at which the flame touches the sidewalls ($\tau_{w,calc}$). As in Figure 3, the data corresponds to closed and half-open ducts for some air-fuel mixtures.

Figure 4 (a) shows correlations for a premixed flame of acetylene in air, inside a closed duct, for an equivalence ratio ranging from 0.40 to 1.70. The value of the Person's coefficient (R^2) was 0.6488, which is an acceptable correlation between the parameters. In Figure 4 (b) the data correspond to a closed duct, the fuel was methane, and the equivalence ratio ranged from 0.72 to 1.30. The value of the Person's coefficient (R^2) was 0.9578, which is a very good correlation between the parameters. The data shown in Figure 4 (c) was obtained in a closed duct, the fuel was a mixture of $0.5H_2+0.5CO$, and the equivalence ratio ranged from 1.0 to 3.0. It is observed that the R^2 coefficient was 0.9517, which denotes an excellent correlation.

Figure 4 (d) shows data for a half-open duct, the fuels were H_2+CO mixtures, the equivalence ratio was 0.80 and the hydrogen fractions ranged from 0.1 to 0.9. The value of the Person's coefficient (R^2) was 0.9427, which is an excellent correlation between the parameters. Figure 4 (e) shows the data obtained for a half-open duct, the fuel was a mixture of H_2+CO mixtures, the equivalence was 1.20, and the hydrogen fractions ranged from 0.1 to 0.9. It is observed that the value of the Person's coefficient (R^2) was 0.995, which is an excellent correlation between the parameters. Finally, in Figure 4 (f) the data correspond to a half-open duct, the fuel was $0.5H_2+0.5CO$, the equivalence ratio ranged from 0.80 to 3.00. The value of the R^2 coefficient was 0.9272, which denotes a very good correlation.

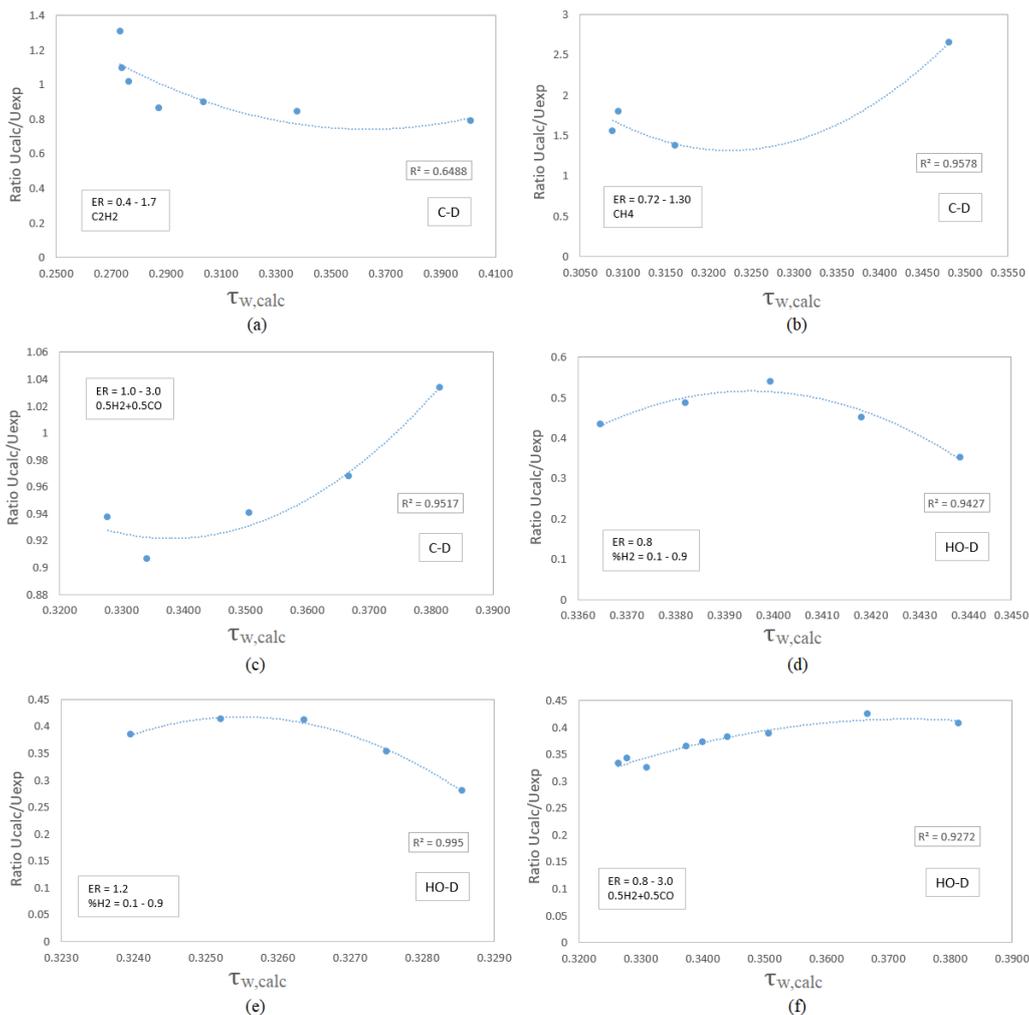


Figure 4. The ratio of maximum velocity U_{calc}/U_{exp} as a function of the time at which the flame touches the sidewalls $\tau_{w,calc}$ in fuel-air mixtures inside closed ducts (a-c) and half-open ducts (d-f).

From the results depicted in Figure 4 it can be concluded that the best correlations for the ratio of U_{calc}/U_{exp} , as a function of the calculated time at which the flame touches the sidewalls ($\tau_{w,calc}$), were obtained for methane and H₂+CO mixtures inside a closed duct, and for H₂+CO mixtures with hydrogen fractions ranging from 0.1 to 0.9 and different equivalence ratios inside a half-open duct. Acetylene showed the lowest correlation coefficient.

As a final step, the experimental and calculated times at which the flame skirt touches the sidewalls are compared in Figure 5 for different fuels and different experimental configurations. In Figure 5 (a) the fuel was methane, and the equivalence ratio ranged from 0.61 to 1.36. It can be observed that the $\tau_{w,exp}$ and $\tau_{w,calc}$ parameters follow a different trend. However, quantitatively the values are well approximated. In Figure 5 (b) the fuel was acetylene and the equivalence ratios ranged from 0.40 to 1.70. It can be observed that $\tau_{w,exp}$ and $\tau_{w,calc}$ follow the same trend. However, quantitatively the results are more distant. In Figure 5 (c) the selected fuel was a mixture of 0.5H₂+0.5CO, the equivalence ratio ranged from 0.80 to 3.00. It can be noticed that $\tau_{w,exp}$ and $\tau_{w,calc}$ follow the same trend. However, the quantitative agreement is not as good as in the first case.

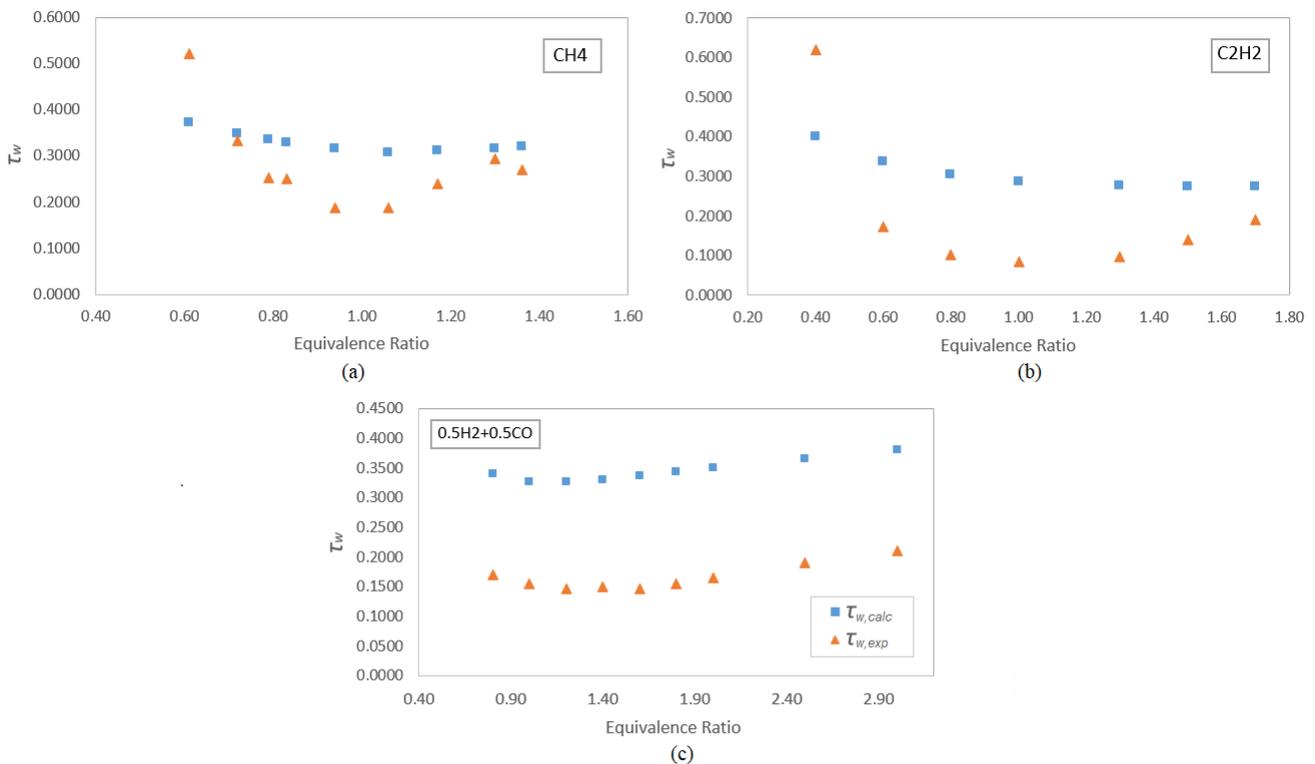


Figure 5. Time of the flame surface reaching the sidewalls (τ_w) for different type of fuels.

From the results obtained above it can be observed that the $\tau_{w,calc}$ has a good qualitative agreement with the $\tau_{w,exp}$, obtained from the experimental works by Jin *et. al.* (2017) and Yang *et. al.* (2020). However, the results do not have a good quantitative agreement. It can be observed that the results of $\tau_{w,calc}$ range from 0.3 to 0.4 regardless of the composition of the fuel mixture. Nevertheless, experimental results show that the composition of the fuel mixture influences the time at which the flame touches the sidewalls (τ_w). Therefore, the determination of τ_w by the available theory is not as accurate as expected. The divergence between the calculated and experimental τ_w is related to the fact that Eq. (2) considers only the expansion ratio and does not capture the effect of the laminar flame speed of the fuel-air mixtures.

From the results presented in this section, it can be observed that the theory proposed by Valiev *et. al.* (2013) worked very well for hydrogen and carbon monoxide mixtures for the determination of the maximum flame tip velocity by using the experimental dimensionless flame tip position at the instant when the flame touches the sidewalls (ξ_{exp}). The consistency of the theory was also tested by comparing the correlation of the maximum velocity ratio (U_{calc}/U_{exp}) and the laminar flame speed (S_L). Also, the correlation between the maximum velocity ratio (U_{calc}/U_{exp}) and the calculated dimensionless time at which the flame skirt touches the sidewalls ($\tau_{w,calc}$) was evaluated. The analysis showed a good correlation between these parameters for different fuels and different equivalence ratios for half-open ducts. In the case of closed ducts, the correlation was acceptable. These results show that the theory is consistent with the experimental data.

4. CONCLUSIONS

In this work, the available theory by Valiev *et al.* (2013) was validated with experimental data published after the publication of that theory. Available data from experimental works were used to verify the correlations between the maximum flame tip flame velocity (U), versus the equivalence ratio, for some air-fuel mixtures. The best agreement was obtained when ξ_{exp} was used, instead of ξ_{calc} , to determine U_{calc} . Therefore, the determination of ξ_{calc} by the theory of Valiev *et al.* (2013) is a key step that causes most of the divergences with the experimental values of the maximum flame tip velocity. For the most part, the results of U_{exp} and $U_{calc}(\xi_{exp})$ had a good agreement quantitatively and qualitatively.

Deflagrations of hydrogen-carbon monoxide mixtures inside closed and half-open ducts were considered, the correlation between the ratio U_{calc}/U_{exp} and the laminar flame speed was analyzed. It was observed that the correlation coefficient shows good results in general. The Pearson's coefficients were 0.7076 and 0.8731 for closed ducts and 0.9213, 0.9754, and 0.9855 for half-open ducts. From the results presented it can be observed that the theory is more accurate for half-open ducts. The theory developed by Valiev *et al.* (2013) did not consider the compression caused by the closed duct configuration. Therefore, the results are coherent with the theoretical boundary conditions. However, the theory shows acceptable agreement when applied to closed ducts.

When the ratio of the maximum flame tip velocity U_{calc}/U_{exp} was plotted as a function of the time at which the flame skirt touched the sidewalls (τ_w) the results showed a very good correlation for hydrogen-carbon monoxide mixtures inside closed and half-open ducts. The Pearson's coefficients varied from 0.9272 to 0.9950. However, when acetylene was considered, the correlation coefficient value was 0.6488.

The comparison of the experimental ($\tau_{w,exp}$) and calculated ($\tau_{w,calc}$) times at which the flame skirt touches the sidewalls have a good qualitative agreement for acetylene and hydrogen-carbon monoxide mixtures when the experimental data, obtained by Jin *et al.* (2017) and Yang *et al.* (2020), were considered. However, the results do not have a good quantitative agreement. It can be observed that the results of $\tau_{w,calc}$ range from 0.3 to 0.4 regardless of the composition of the fuel mixture. The divergence between the calculated and experimental τ_w is related to the fact that Eq. (2) considers only the expansion ratio and does not capture the effect of the laminar flame speed of the fuel-air mixtures.

5. ACKNOWLEDGEMENTS

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